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Directed Graph Evolution from Euler-Lagrange Dynamics

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***Abstract*—In this paper, we develop a variational principle from the von Neumann entropy for directed graph evolution. We minimise the change of entropy over time to investigate how directed networks evolve under the Euler-Lagrange equation. We commence from our recent work in which we show how to compute the approximate von Neumann entropy for a directed graph based on simple in and out degree statistics. To formulate our variational principle we commence by computing the directed graph entropy difference between different time epochs. This is controlled by the ratios of the in-degree and out-degrees at the two nodes forming a directed edge. It also reveals how the entropy change is related to correlations between the changes in-degree ratio and in-degree, and their initial values. We conduct synthetic experiments with three widely studied complex network models, namely Erdős-Rényi random graphs, Watts-Strogatz small-world networks, and Barabási-Albert scale-free networks, to simulate the in-degree and out-degree distribution. Our model effectively captures the directed structural transitions in the dynamic network models. We also apply the method to the real-world financial networks. These networks reflect stock price correlations on the New York Stock Exchange(NYSE) and can be used to characterise stable and unstable trading periods. Our model not only effectively captures how the directed network structure evolves with time, but also allows us to detect periods of anomalous network behaviour.**

1. Introduction

Many real-world complex networks, such as financial networks, communication networks and social networks, change their structure with time. There is an increasing number of studies to develop models analysing the network evolution [1]. Broadly speaking, this problem can be addressed from two different perspectives. The first develops the microscopic approaches to the global characterization of network structure, while the second applies the microscopic description to simulate the local structure of networks. Specifically, at the global level, the function of a network captures the structural variance during the evolution, which can be used to distinguish different types of networks. For example, thermodynamic analysis of network structure describes network structure in terms of macroscopic variables such as temperature. This analysis associates the internal structure to the global pattern of network evolution [8]. On the other hand, at the local level, networks grow and evolve with the addition of new components and connections, or the rewiring of connections from one component to another [7], [11]. Generative and autoregressive models, for example, estimate the detailed evolution of edge connectivity structure with time [2], [8].

However, both the global and the local methods require us to fit the models to the available graph time series data by estimating their parameters. The underlying descriptions of how vertices interact to give edge connections are not simple and difficult to use effectively to simulate network evolution. Motivated by the need to fill this gap in the literature and to augment the methods available for understanding the evolution of time-varying networks, there have been a number of attempts to extend the scope of probabilistic generative models [3], [4]. These models are again highly parameter intensive.

Our recent work has addressed the problem using a generative model of graph-structure [3]. It can be applied to the time-serial networks with an autoregressive model [4]. The key element is the approximate von Neumann entropy on graphs. This entropy is the extension of the Shannon entropy defined over the re-scaled eigenvalues of the normalised Laplacian matrix. A quadratic approximation of the von Neumann entropy gives a simple expression for the entropy associated with the degree combinations of nodes forming edges [6], [8]. Moreover, the fitting of the generative model to dynamic network structure involves a description length criterion which describes both the likelihood of the goodness of fit to the available network data together with the approximate von Neumann entropy of the fitted network. This latter term regulates the complexity of the fitted structure [1], [4], and mitigates against overfitting of the irrelevant or unlikely structure. The change in entropy of the two vertices forming an edge between different epochs depends on the product of the degree of one vertex and the degree change of the second vertex. In other words, the change in entropy depends on the structure of the degree change correlations.

The aim of this paper is to explore whether our model of network entropy can be extended to model the way in which the node degree distribution evolves with time, taking into account the effect of degree correlations caused by the degree structure of directed edges. We focus on the directed graphs and consider the cases where there is a) a mixture of unidirectional and bidirectional edges, b) where the unidirectional edges dominate (strongly directed graphs) and c) where the bidirectional edges outnumber the unidirectional edges (weakly directed graphs). We exploit this property by modelling the evolution of network structure using the Euler-Lagrange equations. Our variational principle is to minimise the changes in entropy during the evolution. Using our approximation of the von Neumann entropy, this leads to update equations for the node degree which include the effects of the node degree correlations induced by the edges of the network. Here we mainly focus on the strongly directed graphs, where edges are purely unidirectional and there are no bi-directional edges. Our model distinguishes between the in-degree and out-degrees of vertices, and it is effectively a type of diffusion process that models how the degree distribution propagates across the network. In fact, it has elements similar to preferential attachment [11], since it favours edges that connect high degree nodes [5], [13].

The remainder of the paper is organized as follows. In Sec. II, we provide a detailed preliminary analysis of network entropy. In Sec. III, We theoretically analyse directed networks with dynamic entropy changes and develop models for degree statistics by minimising the von Neumann entropy change using the Euler-Lagrange equations. In Sec. IV, we conduct numerical experiments on the synthetic and real-world time-varying networks and apply the resulting characterization of network evolution. Finally, we conclude the paper and make suggestions for future work.

2. Network Entropy

Consider a directed graph with node-set V and directed edge-set E. In a recent paper we have shown how to compute an approximtion to the von Neumann entropy for such a graph using just the in-degrees and out-degree of its nodes [10]. To do this we distinguish between two subsets of edges E_1 and E_2, where $E_1 = \{(u,v)|(u,v) \in E \text{ and } (v,u) \notin E\}$ is the set of unidirectional edges, $E_2 = \{(u,v)|(u,v) \in E \text{ and } (v,u) \in E\}$ is the set of bidirectional edges. The two edge-sets satisfy the conditions $E_1 \cup E_2 = E, E_1 \cap E_2 = \emptyset$. With this distinction between unidirectional and bidirectional edges, the approximation for the von Neumann entropy of the directed graph is,

$$S_d = 1-\frac{1}{|V|}-\frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{d_u^{in}}{d_v^{in}d_u^{out^2}}+\sum_{(u,v)\in E_2}\frac{1}{d_u^{out}d_v^{out}}\right\} \tag{1}$$

where d_u^{in} is the in-degree or number of directed edges incoming edges at node u and d_u^{out} is the corresponding out-degree or number of nodes exiting the node.

To simplify the expression according to the relative importance of the sets of unidirectional and bidirectional edges E_1 and E_2, the von Neumann entropy can be further approximated to distinguish between weakly and strongly directed graphs. For weakly directed graphs, i.e., $|E_1| \ll |E_2|$ most of the edges are bidirectional, and we can ignore the summation over E_1 in Eq.(1), rewriting the remaining terms in curly brackets as

$$S_{wd} = 1-\frac{1}{|V|}-\frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{\frac{d_u^{in}}{d_u^{out}}+\frac{d_v^{in}}{d_v^{out}}}{d_u^{out}d_v^{in}}\right\} \tag{2}$$

For the strongly directed graph the unidirectional edges dominate, i.e., $|E_1| \gg |E_2|$, there are few bidirectional edges, and we can ignore the summation over E_2 in Eq.(1), giving the approximate entropy as

$$S_{sd} = 1-\frac{1}{|V|}-\frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{d_u^{in}}{d_v^{in}d_u^{out^2}}\right\} \tag{3}$$

Thus, both the strongly and weakly directed graph entropies depend on the graph size and the in-degree and out-degree statistics of edge connections [10].

3. Variational Principle on Graphs

3.1. Euler-Lagrange Equation

We would like to understand the dynamics of a directed network which evolves so as to minimise the entropy change between different sequential epochs. To do this we cast the evolution process into a variational setting of the Euler-Lagrange equation, and consider the system which optimises the functional

$$\mathcal{E}(q) = \int_{t_1}^{t_2} \mathcal{G}\left[t, q(t), \dot{q}(t)\right] dt \tag{4}$$

where t is time, $q(t)$ is the variable of the system as a function of time, and $\dot{q}(t)$ is the time derivative of $q(t)$. Then, the Euler-Lagrange equation is given by

$$\frac{\partial \mathcal{G}}{\partial q}\left[t, q(t), \dot{q}(t)\right] - \frac{d}{dt}\frac{\partial \mathcal{G}}{\partial \dot{q}}\left[t, q(t), \dot{q}(t)\right] = 0 \tag{5}$$

Here we consider an evolution which changes just the edge connectivity structure of the vertices and does not change the number of vertices in the graph. As a result, the factors $1-\frac{1}{|V|}$ and $\frac{1}{|V|^2}$ are constants and do not affect the solution of the Euler-Lagrange equation.

Consider two nodes u and v forming a directed edge. The ratio of in-degree to out-degree at node u is $r_u = \frac{d_u^{in}}{d_u^{out}}$ and $r_v = \frac{d_v^{in}}{d_v^{out}}$ at node v. We use these node degree ratios to re-write the strongly and weakly directed graph entropies.

3.2. Weakly Directed Graphs

Using the node degree ratios, the weakly directed graph entropy becomes

$$S_{wd} = 1-\frac{1}{|V|}-\frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{r_u(r_u+r_v)}{d_u^{in}d_v^{in}}\right\} \tag{6}$$

As a result, for two weakly directed graphs $G_{wd}^t = (V_t, E_t)$ and $G_{wd}^{t+1} = (V_{t+1}, E_{t+1})$, representing the structure of a time-varying complex network at two consecutive epochs t and $t+1$ respectively, the change of von Neumann entropy is given by

$$\begin{aligned}\Delta S_{wd} &= S(G_{wd}^{t+1}) - S(G_{wd}^t) \\ &= -\frac{1}{2|V|^2}\sum_{(u,v)\in E,E'}\left\{\frac{(2r_u+r_v)\Delta r_u + r_u\Delta r_v}{d_u^{in}d_v^{in}}\right. \\ &\quad \left. - \frac{r_u(r_u+r_v)(d_u^{in}\Delta_v^{in}+d_v^{in}\Delta_u^{in})}{(d_u^{in}d_v^{in})^2}\right\}\end{aligned} \tag{7}$$

where Δ_u^{in} is the change of in-degree for node u, i.e., $\Delta_u^{in} = d_u^{in}(t+1) - d_u^{in}(t)$; Δ_v^{in} is similarly defined as the change of in-degree for node v, i.e., $\Delta_v^{in} = d_v^{in}(t+1) - d_v^{in}(t)$, and Δr_u and Δr_v are the change of in to out degree ratio for the node u and node v respectively.

The Euler-Lagrange equation for r_u gives

$$\frac{\partial \Delta S_{wd}}{\partial \Delta r_u} - \frac{d}{dt}\frac{\partial \Delta S_{wd}}{\partial \Delta r_u} = -\frac{2(2r_u + r_v)(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in}d_v^{in})^2} = 0 \tag{8}$$

and similarly for r_v gives

$$\frac{\partial \Delta S_{wd}}{\partial \Delta r_v} - \frac{d}{dt}\frac{\partial \Delta S_{wd}}{\partial \Delta r_v} = -\frac{2r_u(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in}d_v^{in})^2} = 0 \tag{9}$$

Combining the Eq.(8) and Eq.(9), the relationship between d_u^{in} and d_v^{in} is

$$\frac{\Delta_u^{in}}{d_u^{in}} = -\frac{\Delta_v^{in}}{d_v^{in}} \tag{10}$$

Thus, for the weakly directed graph, there exists a linear correlation between Δ_u^{in}/d_u^{in} and Δ_v^{in}/d_v^{in}.

3.3. Strongly Directed Graphs

For a strongly directed graph, on the other hand, when re-expressed in terms of the node degree ratios, the von Neumann entropy in Eq.(2) becomes

$$S_{sd} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{r_u^2}{d_u^{in}d_v^{in}}\right\} \tag{11}$$

For two strongly directed graphs $G_{sd}^t = (V_t, E_t)$ and $G_{sd}^{t+1} = (V_{t+1}, E_{t+1})$, the change of von Neumann entropy is

$$\begin{aligned}\Delta S_{sd} &= S(G_{sd}^{t+1}) - S(G_{sd}^t) \qquad (12)\\ &= -\frac{1}{2|V|^2}\sum_{(u,v)\in E,E'}\frac{d_u^{in}d_v^{in}\Delta r_u - r_u(d_v^{in}\Delta_u^{in} + d_u^{in}\Delta_v^{in})}{(d_u^{in}d_v^{in})^2}\end{aligned}$$

where Δ_u^{in} is the change of in-degree for node u; Δ_v^{in} is similarly defined as the change of in-degree for node v.

The structure of the above expression deserves further comment. The change in entropy gauges the correlations between the in-degree and node degree changes and in-degrees and in/out degree ratios of the nodes defining the directed edges.

Now we again apply the Euler-Lagrange equation to the changes of entropy for strongly directed graph. The partial derivative of the ratio r_u is

$$\frac{\partial \Delta S_{sd}}{\partial r_u} = -\frac{d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in}}{(d_u^{in}d_v^{in})^2} \tag{13}$$

And the partial time derivative to the first order ratio difference Δr_u is

$$\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} = \frac{2}{d_u^{in}d_v^{in}} \tag{14}$$

Then, the solution of the Euler-Lagrange equation for r_u can be computed as

$$\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} - \frac{d}{dt}\frac{\partial \Delta S_{sd}}{\partial \Delta r_u} = -\frac{2(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in})}{(d_u^{in}d_v^{in})^2} = 0 \tag{15}$$

Similarly, applying the Euler-Lagrange equation on the in-degree d_u^{in}, we get

$$\begin{aligned}&\frac{\partial \Delta S_{sd}}{\partial d_u^{in}} - \frac{d}{dt}\frac{\partial \Delta S_{sd}}{\partial \Delta_u^{in}} = \qquad (16)\\ &\frac{r_u(d_u^{in}\Delta_v^{in} + d_v^{in}\Delta_u^{in}) + d_v^{in}(r_u\Delta_u^{in} - 2d_u^{in}\Delta r_u)}{(d_u^{in})^3(d_v^{in})^2} = 0\end{aligned}$$

Substituting Eq.(15) into Eq.(16), the relationship between d_u and r_u can be obtained

$$\frac{\Delta_u^{in}}{d_u^{in}} = 2\frac{\Delta r_u}{r_u} \tag{17}$$

Therefore, the Euler Lagrange dynamics leads to a linear relationship between $\frac{\Delta_u^{in}}{d_u^{in}}$ and $\frac{\Delta r_u}{r_u}$ for strongly directed graphs. This should be compared to the analogous relationship which arises from the incremental analysis of the ratio $r_u = \frac{d_u^{in}}{d_u^{out}}$,

$$\Delta r_u = \frac{\Delta_u^{in}}{d_u^{out}} - \frac{d_u^{in}\Delta_u^{out}}{(d_u^{out})^2} \tag{18}$$

and as a result

$$\frac{\Delta r_u}{r_u} = \frac{\Delta_u^{in}}{d_u^{in}} - \frac{\Delta_u^{out}}{d_u^{out}} \tag{19}$$

Combining with Eq.(17) gives the growth equation

$$\frac{\Delta_u^{out}}{d_u^{out}} = \frac{1}{2}\frac{\Delta_u^{in}}{d_u^{in}} \tag{20}$$

which is the out-degree grows at half the rate of the in-degree. In the next section we explore empirically how well this relationship is observed.

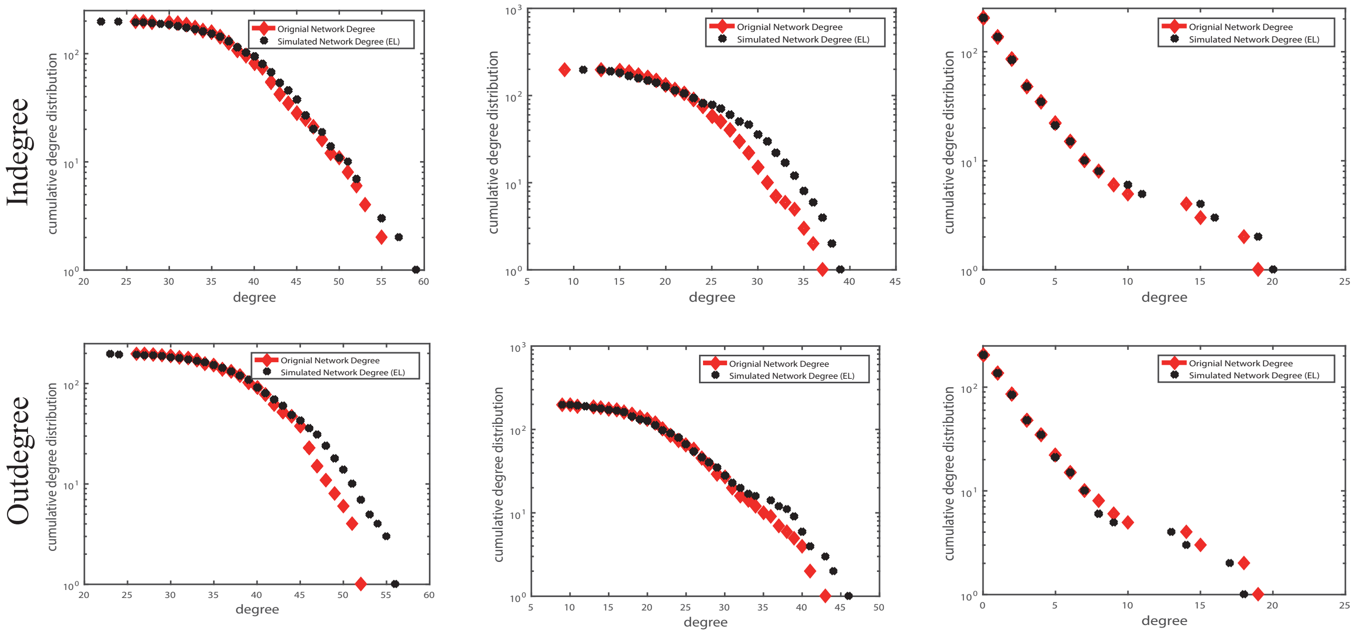
4. Experiments

Here, we use both synthetic and real-world network datasets. The synthetically generated data consists of artificial networks, generated according to a) the Erdős-Rényi random graph model, b) the small world network model and c) the scale-free network model. These represent the three most widely used models of network structure. In addition, we use networks representing daily trading patterns on the New York Stock Exchange.

4.1. Data Sets

Synthetic Networks: We generate graphs according to the three complex network models, namely, a) Erdős-Rényi random graph model, b) Watts-Strogatz small-world model [12], and c) Barabási-Albert scale-free model [11]. These are graphs are created with a fixed number of vertices with time-varying network parameters. For the Erdős-Rényi random graph, the connection probability monotonically increases at the uniform rate of 0.005 per unit time. Similarly, the link rewiring probability in the small-world model [12] increases uniformly between 0 to 1 as the network evolves. For the scale-free model [11], one vertex is added to the connection at each time step.

Real-world Networks: We test our method on data provided by the New York Stock Exchange. This dataset consists



(a) Random Graph (b) Small-world Network (c) Scale-free Network

Figure 1. In-degree and out-degree distribution of original networks and simulated networks for three network models. The red line is for the originally observed networks and the black line is for the results simulated from the Euler-Lagrange analysis. (Erdős-Rényi random graphs, Watts-Strogatz small-world networks, Barabási-Albert scale-free networks.

of the daily prices of 3,799 stocks traded continuously on the New York Stock Exchange over 6000 trading days. The stock prices were obtained from the Yahoo! financial database [14]. A total of 347 stock were selected from this set, for which historical stock prices from January 1986 to February 2011 are available. In our network representation, the nodes correspond to stock and the edges indicate that there is a statistical similarity between the time series associated with the stock closing prices [14].

4.2. Simulation Results

We first conduct experiments on the synthetic networks. We generate three kinds of time-evolving network models from Erdős-Rényi random graphs, Watts-Strogatz small-world networks, and Barabási-Albert scale-free networks to compare with our theoretical analysis.

We aim to determine whether the networks evolve in a manner that is consistent with the principle of minimum entropy change under the Euler-Lagrange equation. We thus turn our attention to how the structure of the synthetic network data changes with time. For the evolution of the three complex network models, we fix the number of vertices to 200. The random graphs evolve from an initially sparse set of edges with a low value of the connection probability to one with a high density of connections with giant connected components. This transition can be observed as we increase the probability of connection. A similar process occurs in the Watts-Strogatz small-world model. As the rewiring probability evolves with time, the network structure changes from a regular ring lattice to a small-world structure with high rewiring probability, and finally becomes an Erdős-Rényi random graph with unit rewiring probability. For the scale-free network, the evolution takes place via preferential attachment. The nodes with the highest degree have the largest probability to receive new links. This process produces several high degree nodes or hubs in the network structure.

Fig.1 compares the in-degree and out-degree distribution from the original time series to the simulation results from the Euler-Lagrange equation. Our model uses the relationship in Eq.(20) to simulate the network structure at different time steps in the evolution of the degree distribution. The in-degree and out-degree distributions resulting from Euler-Lagrange dynamics at the final time step fit quite well to those predicted from the originally observed distributions. This provides empirical evidence that the Euler-Lagrange equation accurately predicts the short-term time evolution of the different network models.

4.3. Directed Financial Networks

Now we turn our attention to the directed graph representation of the New York Stock Exchange data. To extract directed graphs from the stock times series data we compute the correlation of the closing price time series with a time lag. We measure the correlation over 30-day windows separated by a time and then select the lag that results in the maximum correlation. The sign of the lag determines the directionality of the edge. We determine the directionality of the edges using the sign of the lag. All the resulting edges are unidirectional. We, therefore, explore how the time evolution follows our model for strongly directed graphs.

First, we investigate how the distribution of r_u evolves with time. Fig.2 shows the distribution at three different time

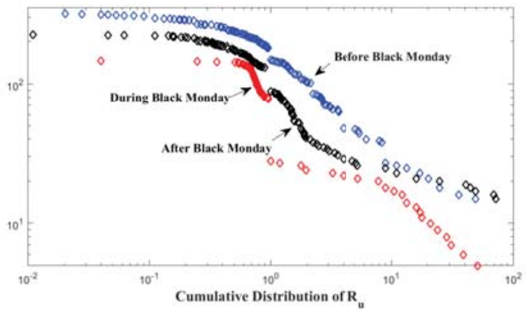


Figure 2. The cumulative distribution of parameter r_u in the directed financial networks before/during/after the Black Monday. The distribution shrinks during the Black Monday crisis.

epochs, i.e., before, during and after Black Monday. Here, the parameter r_u reveals the relationship between in-degree and out-degree for each vertex. As shown in Fig.2, during the Black Monday, the cumulative distribution becomes concentrated over a small range of values around unity. This reflects the fact that a substantial fraction of vertices become isolated during the Black Monday, without out-edges. The remaining connections exist with a balance between in-degree and out-degree. After Black Monday, the network structure begins to recover as the cumulative distribution widens to return to its previous shape.

From the analysis leading to Eq.(10), there is a linear relationship between the quantities $\frac{r_u}{\Delta r_u}$ and $\frac{d_u^{in}}{\Delta_u^{in}}$. In order to test whether this relationship holds in practice, Fig.5 shows scatter plots of $\frac{r_u}{\Delta r_u}$ versus $\frac{d_u^{in}}{\Delta_u^{in}}$ for epochs before, during and after the Black Monday crisis. This provides evidence that there exists a linear relationship between the fractional in-degree change and the degree ratio change. By fitting a linear regression model to the sequence of scatter plots for the time series, we explore how the slope parameters of the regression line and the regression error evolve with time. Fig.3 shows the linear regression errors, as well as the fitted slope, during the period around Black Monday. Here we provide the regression error, for a) the flexible fitting of the slope and b) the regression for a fixed value of the slope. In the time interval around Black Monday, both the linear regression parameter and its error changes abruptly. This is because there are substantial structural differences in the network evolution. During the Black Monday, many nodes become disconnected and the connected components of vertices become small and fragmented. Only a small number of community structures remain highly inter-connected. During Black Monday itself, although the slope of the regression line is zero, the scatter about the line is relatively small.

Furthermore, the linear regression error sequence for the entire directed financial network time series is shown in Fig.4. The peaks in the regression error correspond closely to the occurrence of different financial crises. This regression analysis of the directed graph data thus provides an effective and efficient means of detecting abnormal structure or behaviour in dynamic networks. The most striking observation is that the largest peaks of regression error can be used to identify financial crises. This shows that the theoretical analysis based on minimising the change of directed entropy is sensitive to

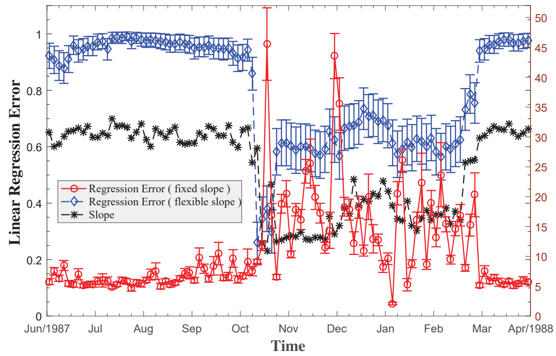


Figure 3. The linear regression error and standard deviation during Black Monday (June 1987 - April 1988). The blue diamond curve is the error bar with the flexible slope of the regression. Red circle line is the errorbar with the fixed slope in the regression. Black star curve is the value of the slope.

significant structural changes in networks. Financial crises are characterized by significant entropy changes, whereas outside these critical periods it remains relatively stable.

5. Conclusion

We use a variational principle based on minimum entropy change to develop a model of network evolution with time. Specifically, we use the Euler-Lagrange equations to minimise the change of von Neumann entropy with time for directed graphs. This treatment leads to a model of how the node degree varies with time and captures the effects of degree change correlations introduced by the edge-structure of the network. We conduct experiments on network time-series representing stock trades on the NYSE. Our model is capable of predicting how the degree distribution evolves with time, provided the trading is not disrupted by financial crises. Moreover, it can also be used to detect abrupt changes in network structure associated with such crises.

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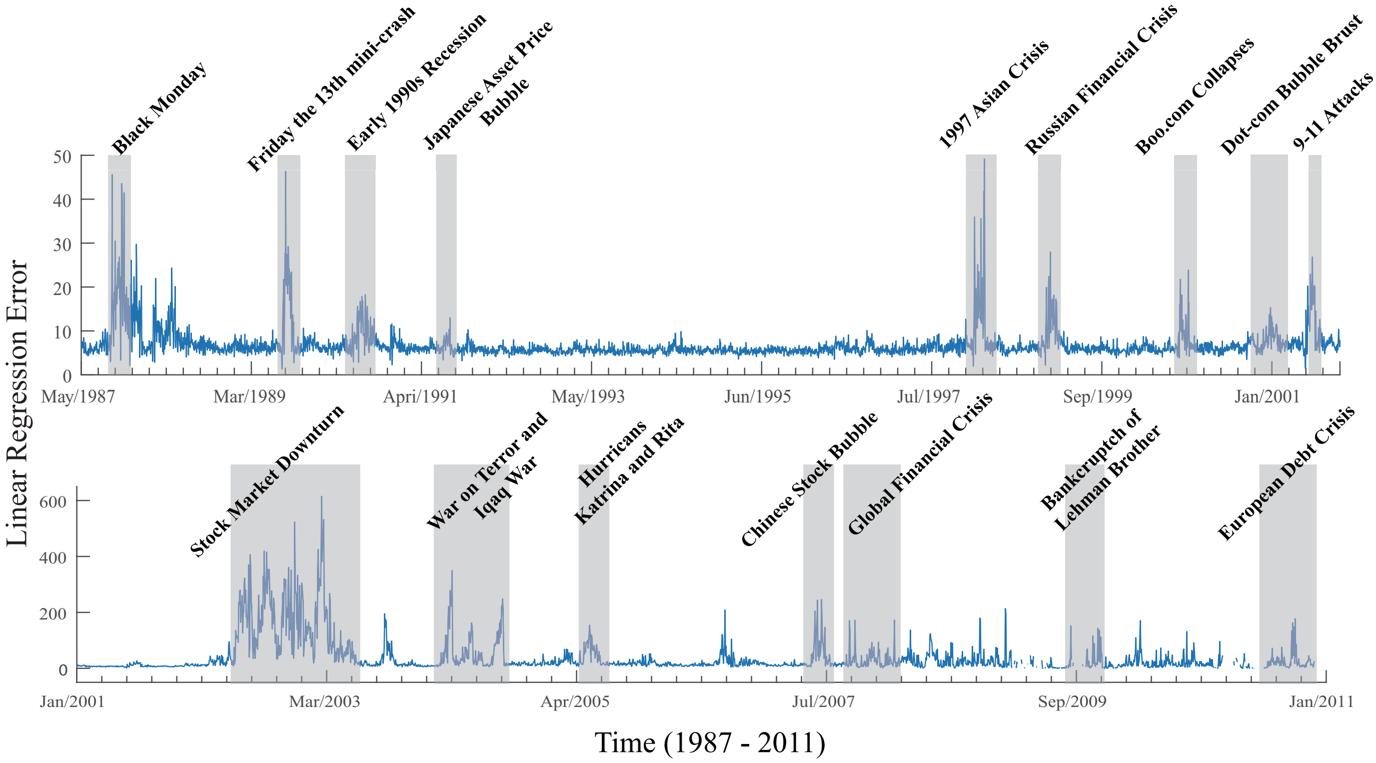

Figure 4. The linear regression error for the whole sequential financial data in NYSE (1987-2011). Critical financial events, i.e., Black Monday, Friday the 13th mini-crash, Early 1990s Recession, 1997 Asian Crisis, 9.11 Attacks, Downturn of 2002-2003, 2007 Financial Crisis, the Bankruptcy of Lehman Brothers and the European Debt Crisis, are associated with significant error peaks.

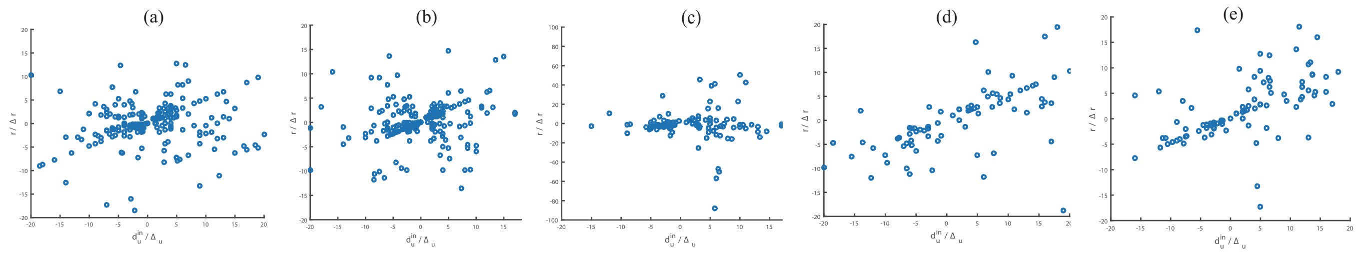

Figure 5. The scatter plots of d_u^{in}/Δ_u^{in} versus $r_u/\Delta r_u$ during the epoch of Black Monday (a)-(e). Before Black Monday: (a) October 1, 1987; (b) October 10, 1987. During Black Monday: (c) October 19, 1987. After Black Monday: (d) October 29, 1987; (e) November 10, 1987

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